arXiv:1004.3422v3 [hep-ph] 16 Aug 2010

Chiral extrapolation and determination of low-energy constants from lattice data[*]

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Abstract

We propose analytic approximations of chiral $SU(3)$ amplitudes for the extrapolation of lattice data to the physical meson masses. The method allows the determination of NNLO low-energy constants in a controllable fashion. We test the approach with recent lattice data for the ratio F_K/F_π of meson decay constants.

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1. Introduction

In recent years, lattice QCD has made enormous progress in the light quark sector (see, e.g., Ref. [1]). State-of-the-art lattice studies employ quark masses corresponding to pion masses as low as 200 MeV, with kaon masses close to the physical value.

Extrapolation to the physical meson masses is performed in different ways. On one side of the theory spectrum, there are various smooth extrapolation formulas with more or less theoretical motivation. On the other side, the most sophisticated extrapolations are based on chiral perturbation theory (CHPT), the effective field theory of the standard model at low energies [2,3]. As the meson masses continue to approach the physical values in future high-statistics simulations[1], even simple-minded polynomial approximations will allow predicting physical quantities with ever better precision. However, a lot of information about QCD is lost in this way. On the other hand, CHPT provides the correct analytic structure of amplitudes in terms of several a priori undetermined constants, the so-called low-energy constants (LECs), which are independent of the light quark masses by definition.

Many of the higher-order LECs are difficult if not impossible to extract from actual experimental data. Lattice calculations offer a new environment for determining LECs because, unlike nature, the lattice physicist can tune the quark masses. For the chiral practitioner, it is then an advantage rather than a drawback that present lattice studies work with different meson masses larger than the physical values.

Many lattice groups use next-to-leading-order (NLO) CHPT results for the chiral extrapolations. As by-products, several LECs at this order, $O(p^4)$, have actually been determined this way (see, e.g., Ref. [5]). On the other hand, state-of-the-art NNLO CHPT results have only very recently been used for the interpretation of lattice data [6–8]. There are good reasons why lattice physicists have generally ignored available NNLO calculations so far: the results are quite involved and, what is even worse, they are mostly available in numerical form only, at least for chiral SU(3) (for a review of NNLO results, see Ref. [9]).

We propose in this note analytic approximations for NNLO CHPT amplitudes for chiral SU(3) that are more sophisticated than the double-log approximation [10], yet much simpler than the full numerical expressions. We first recapitulate CHPT to $O(p^6)$ for the generating functional of Green functions [11]. The form of this functional suggests analytic approximations of p^6-amplitudes that are scale independent in contrast to the double-log approximation. Moreover, they include all leading and next-to-leading contributions at large N_c. In a first exploratory study, we then apply our approximation to the very recent results of the BMW collaboration [12] for the ratio F_K/F_π.

2. Chiral perturbation theory to $O(p^6)$

The most compact representation of CHPT in the meson sector is in terms of the generating functional of Green functions $Z[j]$ [2,3]. In the sequel, we suppress the dependence on external fields j. Analogous to the chiral Lagrangian, the generating functional permits a systematic chiral expansion:

$$Z = Z_2 + Z_4 + Z_6 + \ldots \tag{1}$$

The NNLO functional Z_6 of $O(p^6)$ is itself a sum of different contributions shown pictorially in Fig. 1. In the following, we recapitulate and reformulate the general treatment of

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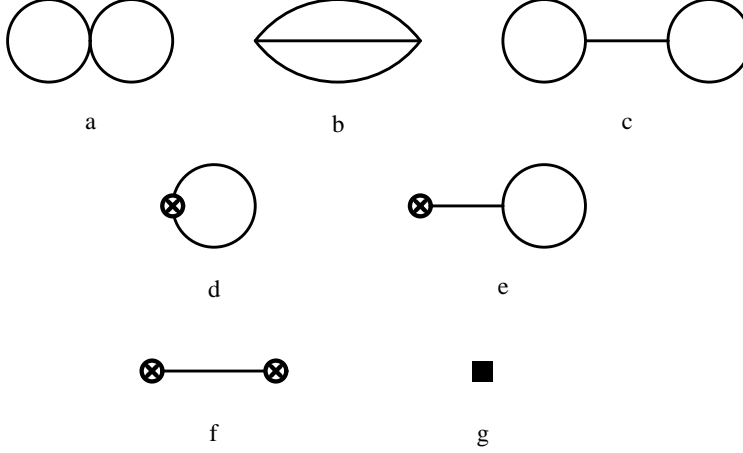[1] A very recent simulation [4] already uses physical quark masses.

Figure 1: Skeleton diagrams for the generating functional Z_6 of $O(p^6)$. Simple dots, crossed circles, black box denote vertices from leading-order, NLO, NNLO Lagrangians, respectively. Propagators and vertices carry the full tree structure associated with the lowest-order Lagrangian.

renormalization at $O(p^6)$ [11]. In addition to tree diagrams of $O(p^6)$ (diagram g), there are two classes of contributions requiring separate treatments: irreducible (diagrams a,b,d) and reducible (diagrams c,e,f) contributions.

With dimensional regularization, the irreducible diagrams have both double- and single-pole divergences. Moreover, the single-pole divergences of each irreducible diagram are in general non-local. Renormalization theory guarantees, however, that the sum of the three diagrams has only local divergences [11, 13], i.e., polynomials in momenta and masses in momentum space. Chiral symmetry guarantees that these divergences can be absorbed by the LECs of $O(p^6)$ via diagram g. In this process an arbitrary renormalization scale μ is generated. The sum of diagrams a,b,d,g is then finite and can be written in the form (details of the derivation will be given elsewhere [14])

$$Z_6^{\mathrm{a+b+d+g}} = \int d^4x \left\{ \left[C_a^r(\mu) + \frac{1}{4F_0^2} \left(4\Gamma_a^{(1)} L - \Gamma_a^{(2)} L^2 + 2\Gamma_a^{(L)}(\mu)L \right) \right] O_a(x) \right.$$

$$\left. + \frac{1}{(4\pi)^2} \left[L_i^r(\mu) - \frac{\Gamma_i}{2} L \right] H_i(x; M) + \frac{1}{(4\pi)^4} K(x; M) \right\} . \tag{2}$$

The structure (2) holds for chiral $SU(n)$ in general but we have already used the notation for $n = 3$. The monomials $O_a(x)$ ($a = 1, \ldots, 94$) define the chiral Lagrangian of $O(p^6)$ [15] with associated renormalized LECs $C_a^r(\mu)$, the $L_i^r(\mu)$ ($i = 1, \ldots, 10$) are renormalized LECs of $O(p^4)$ with associated beta functions Γ_i [3] and the coefficients $\Gamma_a^{(1)}$, $\Gamma_a^{(2)}$ and $\Gamma_a^{(L)}$ are listed in Ref. [11]. Repeated indices are to be summed over. F_0 is the meson decay constant in the chiral $SU(3)$ limit. The chiral log

$$L = \frac{1}{(4\pi)^2} \ln M^2/\mu^2 \tag{3}$$

involves an additional (arbitrary) scale M but $Z_6^{\mathrm{a+b+d+g}}$ as well as the total generating functional are independent of both μ and M. $H_i(x; M)$ are one-loop functionals associated

with diagram d whereas the two-loop contributions (except for the chiral logs) are contained in the functional $K(x; M)$. Unlike $O_a(x)$, the functionals $H_i(x; M)$, $K(x; M)$ are non-local. The scale independence of the functional (2) can be derived with the help of renormalization group equations for the LECs $C_a^r(\mu)$ [11] and $L_i^r(\mu)$ [3], using also relations between the coefficients $\Gamma_a^{(2)}$ and $\Gamma_a^{(L)}$ [11].

As shown in Ref. [11], the sum of reducible diagrams c, e, f gives rise to a finite and scale independent functional with the conventional choice of chiral Lagrangians. It can be written in the form

$$
Z_6^{\text{c+e+f}} = \int d^4x \, d^4y \left[\left(L_i^r(\mu) - \frac{\Gamma_i}{2} L \right) P_{i,\alpha}(x) + F_\alpha(x; M) \right] G_{\alpha,\beta}(x, y)
$$
$$
\left[\left(L_j^r(\mu) - \frac{\Gamma_j}{2} L \right) P_{j,\beta}(y) + F_\beta(y; M) \right] . \tag{4}
$$

Indices α, β run from $1, \ldots, 8$ (octet of pseudoscalar mesons), the $P_{i,\alpha}(x)$ are local functionals, the one-loop contributions of diagrams c,e are contained in the non-local functionals $F_\alpha(x; M)$ and the $G_{\alpha,\beta}(x, y)$ are (functional) propagators.

The complete generating functional of $O(p^6)$ is then given by the sum

$$
Z_6 = Z_6^{\text{a+b+d+g}} + Z_6^{\text{c+e+f}} . \tag{5}
$$

Once again, it is independent of both scales μ and M.

3. Analytic approximation for chiral $SU(3)$

As emphasized in the introduction, the genuine two-loop contributions contained in the functional $K(x; M)$ are usually only available in numerical form for chiral $SU(3)$. On the other hand, the one-loop contributions can be given in analytic form and the dependence on meson masses is manifest. For the chiral extrapolation of lattice results, we therefore suggest the following approximate form for the functional of $O(p^6)$:

$$
Z_6^{\text{app}} = \int d^4x \left\{ \left[C_a^r(\mu) + \frac{1}{4F_0^2} \left(4\,\Gamma_a^{(1)} L - \Gamma_a^{(2)} L^2 + 2\,\Gamma_a^{(L)}(\mu)L \right) \right] O_a(x) \right.
$$
$$
+ \frac{1}{(4\pi)^2} \left[L_i^r(\mu) - \frac{\Gamma_i}{2} L \right] H_i(x; M) \right\}
$$
$$
+ \int d^4x \, d^4y \left\{ \left(L_i^r(\mu) - \frac{\Gamma_i}{2} L \right) P_{i,\alpha}(x) \, G_{\alpha,\beta}(x, y) \left(L_j^r(\mu) - \frac{\Gamma_j}{2} L \right) P_{j,\beta}(y) \right.
$$
$$
\left. + 2 \left(L_i^r(\mu) - \frac{\Gamma_i}{2} L \right) P_{i,\alpha}(x) \, G_{\alpha,\beta}(x, y) \, F_\beta(y; M) \right\} . \tag{6}
$$

In contrast to the generalized double-log approximation [10], which can be recovered by setting the coefficients $\Gamma_a^{(1)}$ and the functionals $H_i(x; M)$, $F_\alpha(x; M)$ to zero, the analytic approximation (6) is scale independent. This is an important asset for a reliable determination of renormalized LECs.

In addition to tabulated quantities [11], the finite and scale independent one-loop functionals $H_i(x; M)$ ($i = 1, \ldots, 10$), $F_\alpha(x; M)$ ($\alpha = 1, \ldots, 8$) must be determined from diagrams

d and e. If available, the corresponding amplitudes can be read off from existing calculations by collecting all amplitudes linear in the LECs $L_i^r(\mu)$.

Another attractive feature of (6) is its large-N_c behaviour. It comprises all leading (generically: C_a, $L_i L_j$) and next-to-leading contributions ($L_i \times$ 1-loop). Of the NNLO terms, it contains at least all chiral logs.

The amplitude for a given observable corresponding to the scale invariant functional (6) can now be determined in four steps.

1. Calculate all tree- and one-loop diagrams, i.e., the contributions from diagrams d,e,f,g in Fig. 1. In many cases of interest, these amplitudes are already available in the literature [9].

2. In the tree-level amplitude of $O(p^6)$ (diagram g), replace the LECs $C_a^r(\mu)$ by

$$C_a^r(\mu) \longrightarrow C_a^r(\mu) + \frac{1}{4F_0^2}\left(4\,\Gamma_a^{(1)}\,L - \Gamma_a^{(2)}\,L^2 + 2\,\Gamma_a^{(L)}(\mu)L\right)\ . \tag{7}$$

We recall that the combination on the right-hand side of (7) is scale invariant.

3. Collect all contributions linear and bilinear in the LECs $L_i^r(\mu)$ in the remaining amplitude (diagrams d,e,f) and extract the chiral logs. The products $L_i^r(\mu)\,L$ from the irreducible parts must match the terms $\Gamma_a^{(L)}(\mu)L$ in (7). After performing this check, set all chiral logs $L = 0$ in this subset of terms (diagrams d,e,f), which amounts to replacing μ by M in the one-loop functions.

4. Replace the bilinears $L_i^r(\mu)L_j^r(\mu)$ (due to reducible contributions: diagram f) by the scale invariant expressions

$$L_i^r(\mu)L_j^r(\mu) \longrightarrow \left(L_i^r(\mu) - \frac{\Gamma_i}{2}L\right)\left(L_j^r(\mu) - \frac{\Gamma_j}{2}L\right)\ . \tag{8}$$

Finally, in the remaining terms linear in the $L_i^r(\mu)$ (originating from diagrams d,e) replace

$$L_i^r(\mu) \longrightarrow L_i^r(\mu) - \frac{\Gamma_i}{2}L\ . \tag{9}$$

The resulting scale invariant amplitude corresponds to the functional (6). The approximation consists in dropping $K(x;M)$ and the terms bilinear in $F_\alpha(x;M)$ in the exact functionals (2) and (4), introducing a dependence on the scale M. This scale parametrizes the two-loop contributions not contained in (6). Transforming the one-loop functionals $H_i(x;M), F_\alpha(x;M)$ back to $H_i(x;\mu), F_\alpha(x;\mu)$, the only M-dependence resides in the chiral logs. The remaining (single and double) chiral logs can then only be due to the two-loop contributions because all other contributions are correctly included in the approximate functional (6) and are therefore independent of M. Experience with the double-log approximation [10] suggests that M is naturally of the order of the kaon mass in $SU(3)$ calculations.

While the above approximation is motivated by large N_c, some of the terms not included in the approximate functional (6) have a relatively simple analytic form (products of one-loop amplitudes from diagrams a,c in Fig. 1). In practice, inclusion of those terms may improve the accuracy of the approximation for certain observables. We will come back to this issue in Ref. [14].

4. Application to lattice data for F_K/F_π

We apply the analytic approximation (6) to the ratio F_K/F_π of meson decay constants. F_K/F_π is well suited for an exploratory study for at least two reasons.

- At the scale $\mu = 0.77$ GeV, the genuine two-loop contribution amounts to -0.005 for physical masses, i.e., half a percent only [6,16].

- The detailed results of the BMW collaboration [12] provide an ideal laboratory for testing our approximation.

The approximate form of F_K/F_π is given in the Appendix where all masses are lowest-order masses of $O(p^2)$ [16,17]. Since we work to $O(p^6)$ the masses in R_4 must be expressed in terms of the lattice masses to $O(p^4)$ [3]. The chiral limit value F_0 is deduced from the experimental value $F_\pi = 92.2$ MeV and physical meson masses, using again the relation to $O(p^4)$ [3].

Here we are mainly interested in getting information on the LECs of $O(p^6)$. Only two combinations of LECs appear: $C_{14} + C_{15}$ and $C_{15} + 2\,C_{17}$. Most of the L_i also contribute to F_K/F_π. Several determinations of the L_i^r are available in the literature [18,19]. All fits of the L_i^r to $O(p^6)$ need to make some assumptions about the C_a^r, in particular for extracting L_5^r from F_K/F_π. L_5 is the only LEC contributing to F_K/F_π at $O(p^4)$. Moreover, L_5^2 appears at $O(p^6)$ to leading order in $1/N_c$. This suggests to fit the lattice data with the three parameters L_5^r, $C_{14}^r + C_{15}^r$ and $C_{15}^r + 2\,C_{17}^r$. For the remaining LECs of $O(p^4)$ we adopt the values of fit 10 of Ref. [18]. Since our approximation is scale independent we may choose the conventional scale $\mu = 0.77$ GeV.

Restricting the data sample of the BMW collaboration [12] to simulation points with $M_\pi < 450$ MeV, we are left with 13 data points. For this exploratory study, we take only the statistical errors of F_K/F_π into account. After all, our main purpose is to investigate the capacity of lattice data for the determination of LECs but not to compete with the detailed analysis of Ref. [12].

Fitting the 13 data points with Eq. (13), we obtain for the LECs at $\mu = 0.77$ GeV

$$
\begin{aligned}
L_5^r &= (0.76 \pm 0.09) \cdot 10^{-3} \\
C_{14}^r + C_{15}^r &= (0.37 \pm 0.08) \cdot 10^{-3} \text{ GeV}^{-2} \\
C_{15}^r + 2\,C_{17}^r &= (1.29 \pm 0.16) \cdot 10^{-3} \text{ GeV}^{-2} \ .
\end{aligned}
\tag{10}
$$

The three parameters are strongly correlated, with correlation coefficients indicated below.

	L_5^r	$C_{14}^r + C_{15}^r$
$C_{15}^r + 2\,C_{17}^r$	0.69	-0.87
L_5^r		-0.95

$$\tag{11}$$

Taking these correlations into account, F_K/F_π for physical meson masses is found to be

$$
F_K/F_\pi = 1.198 \pm 0.005 \ ,
\tag{12}
$$

comparing well with the result $F_K/F_\pi = 1.192(7)_{\text{stat}}(6)_{\text{syst}}$ of Ref. [12]. We stress once more that our errors take only the statistical errors of the lattice values for F_K/F_π into account. The same word of caution applies to $\chi^2/\text{dof} = 1.3$ for the quality of fit.

Although the functional (6) and therefore F_K/F_π in (13) are independent of the renormalization scale μ there is a residual dependence on the scale M of the chiral logs. As announced before, we adopt the natural choice $M = M_K$ (lattice value). Varying this scale by $\pm\,20\,\%$, both F_K/F_π and L_5^r remain practically unchanged while the LECs of $O(p^6)$ vary within two standard deviations. Note that this range for M includes M_η, which is given by the Gell-Mann-Okubo mass formula in the contribution of $O(p^6)$ and is therefore always less than 1.2 M_K for the meson masses under consideration. Taking M too low would enhance the chiral logs too much for an $SU(3)$ observable. The sensitivity to the scale M could be substantially reduced if lattice simulations would use strange quark masses lighter than the physical value. In such a scenario the convergence properties of chiral $SU(3)$ could be improved altogether.

For the case at hand, F_K/F_π and L_5^r are insensitive to the approximation made, with uncertainties determined by lattice errors. The situation is opposite for the LECs of $O(p^6)$: here the approximation errors definitely exceed the lattice errors. The dependence on the other LECs of $O(p^4)$ must be taken into account in addition.

Since C_{15} is subleading in $1/N_c$ our fit determines essentially C_{14} and C_{17} [6]. Although the values depend of course on the input for the L_i^r we have found generically that both C_{14}^r and C_{17}^r are positive and smaller than 10^{-3} GeV^{-2}, always taken at the usual scale $\mu = 0.77$ GeV. Comparing with resonance exchange predictions [20], our results indicate that multi-scalar exchange is important for these LECs. With single resonance exchange only, we would have $C_{14}^R = C_{17}^R < 0$ instead [20]. Our result for L_5^r lies in the range covered by other NNLO fits [18,19].

We cannot compare directly with the results of Bernard and Passemar [6] for $C_{14}^r + C_{15}^r$ and $C_{15}^r + 2C_{17}^r$. First of all, the results of the BMW collaboration were not yet available for their analysis and, what is probably more important, the value of L_5^r was taken as input in Ref. [6]. For the reasons given earlier and because of the strong (anti-)correlations found we consider it more appropriate to fit L_5 together with the LECs of $O(p^6)$. Generically, we find somewhat bigger values for $C_{14}^r + C_{15}^r$ and $C_{15}^r + 2C_{17}^r$ than in Ref. [6].

5. Conclusions

Starting from the structure of the generating functional of Green functions to $O(p^6)$, we have proposed analytic approximations for chiral $SU(3)$ amplitudes that require the calculation of tree-level and one-loop diagrams only. The result serves two purposes:

- It provides flexible and user-friendly extrapolation formulas for lattice data.

- It allows for the determination of higher-order LECs that are otherwise difficult to extract from experimental data.

The approximate amplitudes are independent of the renormalization scale, a prerequisite for a reliable determination of LECs. In addition to including all chiral logs, the amplitudes contain all leading and next-to-leading terms in the $1/N_c$ expansion.

The approach will therefore be especially useful in cases where the genuine two-loop contributions are small, compatible with the large-N_c counting. The ratio F_K/F_π is an interesting observable with this property. Fitting the approximate expression for F_K/F_π to recent lattice data, we obtain a value for F_K/F_π in agreement with the detailed analysis of Ref. [12]. Both F_K/F_π and L_5^r are insensitive to the approximation made. The LECs of

$O(p^6)$, $C_{14}^r + C_{15}^r$ and $C_{15}^r + 2\,C_{17}^r$, are consistent with expectations but subject to uncertainties exceeding the lattice errors.

Although the present study is mainly of exploratory nature we consider the results significant enough to warrant further investigations along these lines [14].

Appendix: Approximate result for F_K/F_π to $O(p^6)$

In the approximation defined by the functional (6), F_K/F_π assumes the following form:

$$F_K/F_\pi \;=\; 1 + R_4 + R_6 \tag{13}$$

$$F_0^2\,R_4 \;=\; 4\,(M_K^2 - M_\pi^2)\,L_5 - 5\,\overline{A}(M_\pi,\mu)/8 + \overline{A}(M_K,\mu)/4 + 3\,\overline{A}(M_\eta,\mu)/8$$

$$
\begin{aligned}
F_0^4\,R_6 \;=\;& 8\,F_0^2(M_K^2 - M_\pi^2)\left(2\,M_K^2\,(C_{14} + C_{15}) + M_\pi^2\,(C_{15} + 2\,C_{17})\right)\\
&+ (M_K^2 - M_\pi^2)\left(-32\,(M_\pi^2 + 2\,M_K^2)L_4\,L_5 - 8\,(3\,M_\pi^2 + M_K^2)L_5^2\right.\\
&\left.\quad + (25\,M_\pi^2 + 17\,M_K^2)L^2/32\right)\\
&+ \frac{(M_K^2 - M_\pi^2)}{(4\pi)^2}\left(-2\,(M_\pi^2 + M_K^2)L_1 - (M_\pi^2 + M_K^2)L_2 - (5\,M_\pi^2 + M_K^2)L_3/18\right.\\
&\quad + 6\,(M_\pi^2 + 2\,M_K^2)L_4 + (14\,M_\pi^2 + 22\,M_K^2)L_5/3 - 12\,(M_\pi^2 + 2\,M_K^2)L_6\\
&\left.\quad + 16\,(M_\pi^2 - M_K^2)L_7 - 4\,(M_\pi^2 + 5\,M_K^2)L_8 + (313\,M_\pi^2 + 271\,M_K^2)L/288\right)\\
&+ 5\,\overline{A}(M_\pi,\mu)^2/8 - \overline{A}(M_K,\mu)^2/8 + \overline{A}(M_\pi,\mu)\,\overline{A}(M_K,\mu)/16\\
&- 3\,\overline{A}(M_\pi,\mu)\,\overline{A}(M_\eta,\mu)/8 - 3\,\overline{A}(M_K,\mu)\,\overline{A}(M_\eta,\mu)/16\\
&+ \overline{A}(M_\pi,\mu)\left(4\,M_\pi^2 L_1 + 10\,M_\pi^2 L_2 + 13\,M_\pi^2 L_3/2 + 10\,(M_\pi^2 + 2\,M_K^2)L_4\right.\\
&\quad + (19\,M_\pi^2 - 5\,M_K^2)L_5/2 - 10\,(M_\pi^2 + 2\,M_K^2)L_6 - 10\,M_\pi^2 L_8\\
&\left.\quad - (361\,M_\pi^2 + 131\,M_K^2)L/288\right)\\
&+ \overline{A}(M_K,\mu)\left(-4\,M_K^2 L_1 - 10\,M_K^2 L_2 - 5\,M_K^2 L_3 - 4\,(M_\pi^2 + 2\,M_K^2)L_4\right.\\
&\left.\quad - (M_\pi^2 + M_K^2)L_5 + 4\,(M_\pi^2 + 2\,M_K^2)L_6 + 4\,M_K^2 L_8 + (59\,M_\pi^2 + 115\,M_K^2)L/144\right)\\
&+ \overline{A}(M_\eta,\mu)(M_K^2 - M_\pi^2)/M_\eta^2\left(-9\,M_\pi^2 L_7 - 3\,M_\pi^2 L_8 + 5\,M_\pi^2 L/32\right)\\
&+ \overline{A}(M_\eta,\mu)\left((M_\pi^2/2 - 2\,M_K^2)L_3 - 6\,(M_\pi^2 + 2\,M_K^2)L_4 - (7\,M_\pi^2 + 23\,M_K^2)L_5/6\right.\\
&\quad + 6\,(M_\pi^2 + 2\,M_K^2)L_6 + 3\,(3\,M_\pi^2 M_K^2/M_\eta^2 - 7\,M_\pi^2 + 4\,M_K^2)L_7\\
&\quad + 3\,(M_\pi^2 M_K^2/M_\eta^2 - 3\,M_\pi^2 + 4\,M_K^2)L_8\\
&\left.\quad - (15\,M_\pi^2 M_K^2/M_\eta^2 - 44\,M_\pi^2 - 19\,M_K^2)L/96\right)
\end{aligned}
$$

The abbreviations $L_i = L_i^r(\mu)$, $C_a = C_a^r(\mu)$ have been used for a compact representation. The masses are the lowest-order meson masses of $O(p^2)$, F_0 is the meson decay constant in the chiral $SU(3)$ limit and the chiral log L is defined in (3). The loop function $\overline{A}(M_\alpha,\mu)$ is defined as

$$\overline{A}(M_\alpha,\mu) = \frac{M_\alpha^2}{(4\pi)^2}\log\frac{\mu^2}{M_\alpha^2}\;. \tag{14}$$

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